Conclusion Notes

**Paragraph 1: What we did and why we did it**

We proposed two computationally tractable methods to conduct analytic inversions to infer high-resolution emissions from satellite observations of atmospheric composition while maximizing information content. The methods decrease computational cost by exploiting the dominant patters of information content in the prior emissions estimate and observations to construct the Jacobian matrix, which represents the sensitivity of simulated atmospheric concentrations to emissions for a given forward model, in a reduced-dimension or reduced-rank emissions space instead of at native resolution. Both methods can be applied more generally to the problem of efficient numerical approximation of high-dimension Jacobian matrices.

**Paragraph 2: Analytic solution to the inverse problem and optimal reductions in dimension and rank**

We considered inverse problems where the forward model is linear with respect to the optimized state vector elements, in our case an emissions grid, and where the errors can be assumed to be normally distributed. In this case, there exists an analytic solution to a Bayesian cost function that yields closed-form characterization of the optimized (posterior) emissions, errors, and information content, given by the averaging kernel matrix. The sum of the diagonal elements of the averaging kernel matrix, called here sensitivities, yields the degrees of freedom for signal (DOFS), the number of pieces of information that can be independently quantified by the inverse system. The analytic solution requires explicit construction of the Jacobian matrix, which is typically constructed by finite difference, requiring a model simulation for every state vector element. When inferring emissions at high resolution, constructing this matrix can become computationally intractable.

The number of model runs needed to construct the Jacobian matrix can be decreased by reducing either the dimension or rank of the state vector space. An optimal dimension- or rank-reduction preserves information content. However, the averaging kernel matrix is a function of the Jacobian matrix. The methods proposed here use a two-step update to improve an initial estimate of the Jacobian matrix and the corresponding averaging kernel matrix. We suggested generating a low-cost initial estimate of the Jacobian matrix using a mass balance approach. Because the averaging kernel matrix has a strong dependence on the prior and observational error covariance matrices, this initial estimate can accurately quantify the fine structure of information content.

**Paragraph 3: Reduced dimension construction**

The reduced-dimension method uses the initial estimate of the averaging kernel matrix to build the Jacobian matrix on a multiscale grid that maintains native resolution where information content is highest and aggregates grid cells elsewhere. The method constructs the multiscale grid and corresponding Jacobian matrix element-by-element, introducing first the native-resolution grid cells with the highest averaging kernel sensitivities. For each added state vector element, the forward model response is calculated and the inversion solved. When the total DOFS stabilize, the process is repeated with clusters of grid cells generated by, for example, K-means clustering. When all native-resolution grid cells are allocated to the multiscale grid and the reduced-dimension Jacobian is constructed, the clusters where the forward model contributed the most information content are disaggregated, generating a second update of the multiscale grid and reduced-dimension Jacobian matrix. The information content from both the first and second update contains contributions from the prior emissions estimate, the observations and the forward model; no further iteration is needed.

**Paragraph 4: Reduced rank construction**

The reduced-rank method constructs an approximation of the Jacobian matrix by calculating the linear relationship between emissions and observations in the forward model for the most important patterns of information content rather than individual or aggregate grid cells. These patterns are given by dimension-reducing and -restoring transformations that best preserve information content introduced by Bousserez and Henze (2018). The number of patterns used can be determined by requiring that the signal-to-noise ratio of each pattern or the fraction of the DOFS explained by the patterns exceed a given threshold. The initial estimate of the averaging kernel matrix is used to calculate those patterns, which are then perturbed in the forward model. The resulting forward model response is transformed back to the native-resolution dimension using the optimal dimension-restoring transformation, generating a reduced-rank approximation of the Jacobian matrix. This process is then repeated using the updated Jacobian matrix and corresponding averaging kernel matrix. As with the reduced-dimension method, we find rapid convergence and no need for further iteration.

**Paragraph 5: Results summary**

We applied both methods in a demonstration inversion of GOSAT column methane observations for July 2009 at 1º x 1.25º resolution over the North American domain. We constructed a native-resolution, reduced-dimension, and reduced-rank Jacobian matrix, solved each inversion, and compared the results. We found that both methods were capable of reducing the computational cost of constructing the Jacobian matrix by 75% while accurately constraining posterior emissions where information content is highest. The reduced-dimension Jacobian solved the inversion exactly on a multiscale grid with dimension 423, including clusters of between 1 and 58 native-resolution grid boxes. While the reduced-dimension inversion produced fewer than half of the native-resolution DOFS, it generated twice the DOFS per state vector element. The reduced-dimension Jacobian solved the inversion accurately in the native-resolution grid boxes with the highest information content, defaulting to the prior emissions estimate elsewhere and preserving 70% of the native-resolution DOFS. Because of the loss of information content, the error of the optimized emissions also increases. The trade-off between resolution and precision

**Paragraph 7: Next steps**

In an era where satellites provide increasingly high-resolution, dense observations of atmospheric constituents, analytic inversions of linear systems can improve constraints on emission sources and characterize the associated errors and information content. Previously, the analytic approach was limited by the computational cost of constructing the Jacobian matrix, which required a forward model simulation for every state vector element constrained by the inversion. Our methods allow analytic inversion of satellite observations at high-resolution with many fewer forward model simulations.